

Crossover between aperiodic and homogeneous semi-infinite critical behaviors in multilayered two-dimensional Ising models

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We investigate the surface critical behavior of two-dimensional multilayered aperiodic Ising models in the extreme anisotropic limit. The system under consideration is obtained by piling up two types of layers with respectively p and q spin rows coupled *via* nearest neighbor interactions λ_r and λ , where the succession of layers follows an aperiodic sequence generated through substitution rules. Far away from the critical regime, the correlation length ξ_{\perp} , measured in lattice spacing units, in the direction perpendicular to the layers is smaller than the first layer width and the system exhibits the usual behavior of an ordinary surface transition. In the other limit, in the neighborhood of the critical point, ξ_{\perp} diverges and the fluctuations are sensitive to the non-periodic structure of the system so that the critical behavior is governed by a new fixed point. We determine the critical exponent associated to the surface magnetization at the aperiodic critical point and show that the expected crossover between the two regimes is well described by a scaling function. From numerical calculations, the parallel correlation length ξ_{\parallel} is then found to behave with an anisotropy exponent z which depends on the aperiodic modulation and the layer widths.

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I. INTRODUCTION

Since the discovery of quasi-crystals,¹ the critical properties of aperiodic systems have been intensively studied (for a review, see Ref. 2). These systems display, in some cases, the same type of singularities which can be encountered in random systems, the study of which is a quite active field of research.

In layered systems, generalizing the McCoy-Wu model,³⁻⁶ aperiodic distributions of the exchange interactions between successive layers in the Ising model have been considered.⁷⁻¹² In Ref. 13, the Onsager logarithmic singularity of the specific heat was found to be washed out. The major result was obtained by Luck,¹⁴ by a generalization to layered perturbations of the Harris criterion for random systems.¹⁵

According to Luck's criterion, aperiodic modulations may be relevant, marginal or irrelevant, depending on the correlation length exponent ν of the unperturbed system, and on a wandering exponent ω which characterizes the fluctuations of the couplings around their average.^{16,17} Systematic studies of the surface critical properties for irrelevant, marginal, and relevant perturbations have been achieved in the extreme anisotropic limit.¹⁸⁻²¹ In the case of bulk marginal sequences (i.e. which modifies both surface and bulk properties), an anisotropic scaling behavior was obtained in the Hamiltonian limit,^{22,23} as well as in the classical two-dimensional counterpart,²⁴ or in hierarchical models.²⁵ In these systems, both surface and bulk properties have been studied and the bulk specific heat exponent, given by $\alpha = 1 - z$, where z is the anisotropy exponent, is always negative leading to a non-diverging singular behavior.

In the present paper, we continue the investigation of the surface critical behavior of marginal sequences,

through a study of the crossover between usual ordinary surface transition and aperiodic critical behavior in multilayered Ising models. Up to now, only layered systems have been considered, and we study here multilayered systems made of the piling up of two kinds of layers of widths p and q . In such systems, together with the perpendicular correlation length ξ_{\perp} , the first layer width p plays the role of a relevant length scale entering the description of the critical behavior in the vicinity of the free surface. Depending on the value of the scaled variable p/ξ_{\perp} , one thus expects a crossover between the two regimes. In section II, we recall some generalities about aperiodic sequences generated through substitution and give a short summary of the relevance criterion proposed by Luck. The critical behavior of the surface magnetization in multilayered models at the aperiodic fixed point is determined in Sec. III and the crossover effect, which constitutes the main result of the paper is presented in Sec. IV. In section V, a numerical study of the parallel correlation length ξ_{\parallel} allows the determination of the anisotropy exponent of multilayered Ising models in agreement with a relation, already established in the layered case, which seemingly has a general field of application.

II. LUCK'S CRITERION

Many results have already been obtained in $2d$ layered Ising models with constant interactions K_1 along the layers and modulated interactions $K_2(k)$ between successive spin rows, k and $k+1$. The transfer matrix should in principle be diagonalized for arbitrary couplings,²⁶ but in the following one considers the extreme anisotropic limit. In the Hamiltonian limit, $K_1 \rightarrow \infty$, $K_2 \rightarrow 0$, while keeping

the ratio $\lambda_k = K_2(k)/K_1^*$ fixed, where $K_1^* = -\frac{1}{2} \ln \tanh K_1$ is the dual coupling, the row-to-row transfer operator $\mathcal{T} = \exp[-2K_1^* \mathcal{H}]$ involves the Hamiltonian of a quantum Ising chain in a transverse field:^{27,28}

$$\mathcal{H} = -\frac{1}{2} \sum_{k=1}^L (\sigma_k^z + \lambda_k \sigma_k^x \sigma_{k+1}^x) , \quad (2.1)$$

where the σ 's are Pauli spin operators.

The Jordan-Wigner transformation,²⁹ followed by a canonical transformation, maps Eq. (2.1) onto a free fermions problem:³⁰

$$\mathcal{H} = \sum_{\alpha} \varepsilon_{\alpha} (\eta_{\alpha}^{\dagger} \eta_{\alpha} - \frac{1}{2}) . \quad (2.2)$$

The fermion excitations ε_{α} follow from the solution of the linear system

$$\begin{aligned} \varepsilon_{\alpha} \Psi_{\alpha}(k) &= -\Phi_{\alpha}(k) - \lambda_k \Phi_{\alpha}(k+1) \\ \varepsilon_{\alpha} \Phi_{\alpha}(k) &= -\lambda_{k-1} \Psi_{\alpha}(k-1) - \Psi_{\alpha}(k) \end{aligned} \quad (2.3)$$

which may be rewritten as a single eigenvalue equation, either for Φ or Ψ which are assumed to be normalized and free boundary conditions $\lambda_0 = \lambda_L = 0$ are imposed.

The surface properties are defined as usually by matrix elements: the surface magnetization m_s is given by $\langle 1 | \sigma_1^x | 0 \rangle$ where $|0\rangle$ is the ground state of \mathcal{H} and $|1\rangle$ is the first excited state. Using the transformation to η -fermionic operators, the surface magnetization takes the simple form $m_s = \Phi_1(1)$. The surface energy density e_s involves the lowest two-fermion excited state $|2\rangle = \eta_1^+ \eta_2^+ |0\rangle$, and can thus be written $e_s = \langle 2 | \sigma_1^z | 0 \rangle = (\varepsilon_2 - \varepsilon_1) \Phi_1(1) \Phi_2(1)$.

With an aperiodic modulation of the couplings, one may write:

$$\lambda_k = \lambda r^{f_k} , \quad (2.4)$$

where f_k , which may be 0 or 1, is determined by the aperiodic sequence. Let $n_L = \sum_{k=1}^L f_k$ be the number of modified couplings on a chain with length L ; their asymptotic density is $\rho_{\infty} = \lim_{L \rightarrow \infty} n_L/L$. The critical coupling λ_c obeys the following condition:³¹

$$\lim_{L \rightarrow \infty} \prod_{l=1}^L (\lambda_l)_c^{1/L} = 1, \quad (2.5)$$

which, using equation (2.4), gives:

$$\lambda_c = r^{-\rho_{\infty}} . \quad (2.6)$$

The sequences considered below are generated through substitutions rules, either on digits (“period-doubling”) or on pairs of digits (“paper-folding”).

The “period-doubling” (PD) sequence^{14,18,20,32} may be defined by the substitutions $\mathcal{S}(0) = 1 \ 1$ and $\mathcal{S}(1) = 1 \ 0$, which, starting on 1, give successively:

$$\begin{aligned} n=1 & \quad 1 \\ n=2 & \quad 1 \ 0 \\ n=3 & \quad 1 \ 0 \ 1 \ 1 \\ n=4 & \quad 1 \ 0 \ 1 \ 1 \ 1 \ 0 \ 1 \ 0 \end{aligned} \quad (2.7)$$

The “paper-folding” (PF) sequence is generated through substitutions on pairs of digits, and details can be found in Ref. 23,33.

Most of the properties of a sequence are obtained from its substitution matrix^{16,17} with entries M_{ij} giving the number $n_i^{\mathcal{S}(j)}$ of digits (or pairs) of type i in $\mathcal{S}(j)$. The asymptotic density of modified interactions, ρ_{∞} , is deduced from the eigenvector corresponding to the leading eigenvalue Λ_1 of the substitution matrix, allowing the calculation of the critical coupling *via* Eq. (2.6). The length of the sequence after n iterations of the substitution rules is asymptotically related to the leading eigenvalue through $L_n \sim \Lambda_1^n$. Finally, the fluctuations of the f_k 's at a length scale L_n are governed by the next-to-leading eigenvalue Λ_2 :

$$\sum_{k=1}^{L_n} f_k \simeq \rho_{\infty} L_n + |\Lambda_2|^n F\left(\frac{\ln L_n}{\ln \Lambda_1}\right) \quad (2.8)$$

where $F(x)$ is a periodic “fractal function”¹⁴ as shown in Fig. 1.

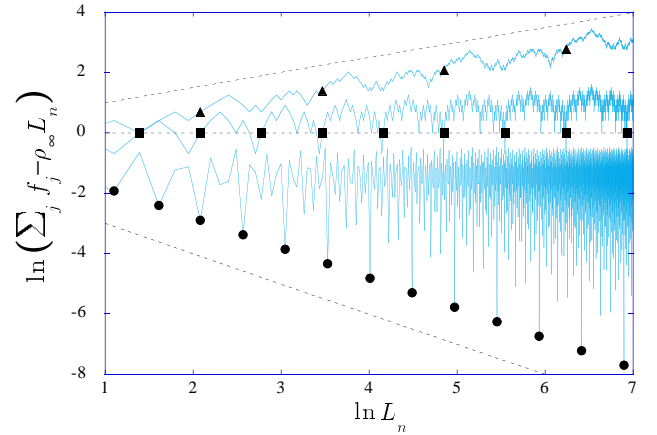


FIG. 1. Fluctuations of the sum of the f_k 's around their average for three different aperiodic sequences (top: Rudin-Shapiro, $\omega = 1/2$; middle: “paper-folding”, $\omega = 0$; bottom: Fibonacci, $\omega = -1$). The symbols correspond to sizes which do respect the symmetries of the chains and the dotted lines have slopes ω .

The cumulated deviation per bond of the couplings from their average $\bar{\lambda}$ is thus written

$$\overline{\delta(L_n)} = \frac{1}{L_n} \sum_{k=1}^{L_n} (\lambda_k - \bar{\lambda}) \sim \delta |\Lambda_2|^n \sim \delta L_n^{\omega} \quad (2.9)$$

where $\delta = \lambda(r - 1)$ is the amplitude of the modulation and ω is the wandering exponent given by:

$$\omega = \frac{\ln |\Lambda_2|}{\ln \Lambda_1}. \quad (2.10)$$

Since the relevant length scale is the correlation length ξ , the aperiodicity thus induces a thermal perturbation

$$\frac{\overline{\delta(\xi)}}{t} \sim t^{-\phi}, \quad \phi = 1 + \nu(\omega - 1) \quad (2.11)$$

involving a crossover exponent ϕ .¹⁴ When $\phi > 0$, the perturbation diverges as $t \rightarrow 0$, corresponding to a relevant perturbation. When $\phi < 0$, the perturbation is washed out when the critical point is approached; it is irrelevant. When $\phi = 0$, the perturbation is marginal and may lead to a non-universal behaviour with perturbation-dependent critical exponents. In the following, we will only consider marginal sequences.

In the case of the 2d Ising model, since $\nu = 1$, the relevance of the perturbation is directly determined by ω as shown in Fig. 1.

III. SURFACE MAGNETIZATION IN MULTILAYERED ISING MODELS

A. Critical point and surface magnetization

The first excited state of the Hamiltonian, $|1\rangle$, is degenerate with the ground state in the ordered phase of the infinite system and, since a simplification occurs in Eq. (2.3) when ε_1 vanishes, the first relation provides a recursion for the components of Φ_1 . After normalization one obtains the surface magnetization of the semi-infinite system as:³⁴

$$m_s = S^{-1/2}, \quad S = 1 + \sum_{j=1}^{\infty} \prod_{k=1}^j \lambda_k^{-2} \quad (3.1)$$

which remains valid for any distribution of the interactions.

We consider here a multilayered Ising model where the aperiodic sequence $f_k = 1, 0, 1, 1 \dots$ refers now to successive layers with $p, q, p, p \dots$ spin rows. A layer labelled by index k contains p (respectively q) exchange interactions λr (respectively λ) between nearest neighbor rows according to the following scheme showing the first three layers:

$$\begin{array}{ccccccc} & \overbrace{\lambda r \quad \lambda r \quad \dots \lambda r}^{p \text{ terms}} & \overbrace{\lambda \quad \lambda \quad \dots \lambda}^{q \text{ terms}} & \overbrace{\lambda r \quad \lambda r \quad \dots \lambda r}^{p \text{ terms}} & & & \\ k & & & & & & \\ f_k & 1 & 0 & 1 & & & \\ l & 1 \ 2 \dots p & p+1 \dots p+q & p+q+1 \dots 2p+q & & & \end{array} \quad (3.2)$$

Let us first determine the critical coupling λ_c . The width of layer k is written

$$m_k = (p - q)f_k + q. \quad (3.3)$$

On the system containing L layers, one has n_L layers of type p and $L - n_L$ of type q and the critical value is still determined through Eq. (2.5) where

$$\prod_{l=1}^L (\lambda_l)_c^{1/L} = (\lambda_c r)^{p n_L / L} (\lambda_c)^{q(L - n_L) / L}. \quad (3.4)$$

In the thermodynamic limit, it yields

$$\lambda_c = r^{-\frac{p p_{\infty}}{(p-q)p_{\infty} + q}}. \quad (3.5)$$

The aperiodic series (3.1) entering the surface magnetization has the form

$$\begin{aligned} S^{(m)}(\lambda, r) = 1 + \sum_{l=1}^{m_1} (\lambda r^{f_1})^{-2l} + (\lambda r^{f_1})^{-2m_1} \sum_{l=1}^{m_2} (\lambda r^{f_2})^{-2l} \\ + (\lambda r^{f_1})^{-2m_1} (\lambda r^{f_2})^{-2m_2} \sum_{l=1}^{m_3} (\lambda r^{f_3})^{-2l} + \dots \end{aligned} \quad (3.6)$$

where the superscript (m) is for the multilayered system. This expression may be shortened with the notations

$$\sigma_k = \sum_{l=1}^{m_k} (\lambda r^{f_k})^{-2l} = \begin{cases} \frac{1 - (\lambda r)^{-2p}}{(\lambda r)^2 - 1} = a_p & \text{if } f_k = 1 \\ \frac{1 - \lambda^{-2q}}{\lambda^2 - 1} = b_q & \text{if } f_k = 0 \end{cases} \quad (3.7)$$

and $g_k = (\lambda r^{f_k})^{-2m_k}$. Equation (3.6) then becomes

$$S^{(m)}(\lambda, r) = 1 + b_q \Sigma(\lambda, r) + (a_p - b_q) \Sigma'(\lambda, r) \quad (3.8)$$

where

$$\begin{aligned} \Sigma(\lambda, r) &= \sum_{j=0}^{\infty} \prod_{k=0}^j g_k, \\ \Sigma'(\lambda, r) &= \sum_{j=0}^{\infty} f_{j+1} \prod_{k=0}^j g_k, \end{aligned} \quad (3.9)$$

and $f_0 \equiv 0$. In the second sum, Σ' , f_{j+1} may be rewritten as

$$f_{j+1} = \frac{(\lambda^{p-q} r^p)^{-2f_{j+1}} - 1}{(\lambda^{p-q} r^p)^{-2} - 1} \quad (3.10)$$

and Eq. (3.8) translates into

$$\begin{aligned} S^{(m)}(\lambda, r) = 1 - \frac{\lambda^{2q}(a_p - b_q)}{(\lambda^{p-q} r^p)^{-2} - 1} \\ + \left[b_q + \frac{(\lambda^{2q} - 1)(a_p - b_q)}{(\lambda^{p-q} r^p)^{-2} - 1} \right] \Sigma(\lambda, r). \end{aligned} \quad (3.11)$$

The critical behavior of the surface magnetization is governed by the sum Σ , for which an identity can be found, relating it to the aperiodic series $S^{(l)}$ of the usual

layered system in the case $p = q = 1$. Taking account of Eq. (2.4), the series $S^{(l)}(\lambda, r)$ in Eq. (3.1) takes the form

$$S^{(l)}(\lambda, r) = \sum_{j=0}^{\infty} \lambda^{-2j} r^{-2n_j} \quad (3.12)$$

where the superscript (l) stands now for the layered problem. One usually studies this expression for specific sequences,^{18,21,23} but for our purpose a more convenient expression can be rewritten as a function of the deviation from the critical point:³⁵

$$t = 1 - \left(\frac{\lambda_c}{\lambda} \right)^2. \quad (3.13)$$

Equation (3.12) becomes

$$\tilde{S}^{(l)}(t, \lambda_c) = \sum_{j=0}^{\infty} (1-t)^j \lambda_c^{-2(j-n_j/\rho_\infty)}. \quad (3.14)$$

The analysis of the sum Σ is now facilitated, since the following identity holds:

$$\Sigma(\lambda, r) = S^{(l)}(\lambda^q, \lambda^{p-q} r^p). \quad (3.15)$$

With the variable t , it becomes

$$\tilde{\Sigma}(t, \lambda_c) = \sum_{j=0}^{\infty} (1-t)^{(p-q)n_j + qj} (\lambda_c^q)^{-2(j-n_j/\rho_\infty)} \quad (3.16)$$

and the critical point behavior reduces to the same series as the layered problem up to the transformation $\lambda_c \rightarrow \lambda_c^q$:

$$\tilde{\Sigma}(0, \lambda_c) = \sum_{j=0}^{\infty} (\lambda_c^q)^{-2(j-n_j/\rho_\infty)} = \tilde{S}^{(l)}(0, \lambda_c^q). \quad (3.17)$$

This expression is the basis of further asymptotic analyses using the scaling method proposed by Iglói.³⁶ Let a power series $M(x)$ have a power law singularity at the transition point $x = x_0$: $M(x) \sim (1 - x/x_0)^\beta$. The truncated series of the first L terms at the critical point thus have the following behavior $M_L(x_0) \sim L^{-\beta}$ which allows the determination of β . Equation (3.17) also holds for the truncated series and leads to a simple relation between the critical exponents of the layered problem and the multilayered one:

$$\beta_s^{(m)}(\lambda_c) = \beta_s^{(l)}(\lambda_c^q). \quad (3.18)$$

B. Period-doubling and paper-folding sequences

The period-doubling sequence, given after several substitutions in Eq. (2.7), corresponds to a vanishing wandering exponent and an asymptotic density of modified couplings $\rho_\infty = 2/3$, leading to the critical coupling for the multilayered Ising model coupling *via* Eq. (3.5):

$$\lambda_c = r^{-\frac{2p}{2p+q}}. \quad (3.19)$$

Equation (3.16) can be rewritten as an infinite product,¹⁸ whose first l terms contain, at the critical point $t = 0$, the first $L = 2^{2l}$ terms of the sum (3.14) which becomes

$$\tilde{\Sigma}_{L=2^{2l}}(0, \lambda_c) = [(1 + \lambda_c^q)(1 + \lambda_c^{-q})]^l \sim (2^{2l})^{2\beta_s^{(m)}}. \quad (3.20)$$

The surface exponent then follows:³⁶

$$\beta_s^{(m)}(\lambda_c) = \frac{\ln[(1 + \lambda_c^q)(1 + \lambda_c^{-q})]}{4 \ln 2}. \quad (3.21)$$

Going back to the original parameters, one finally obtains:

$$\beta_s^{(m)}(r, p, q) = \frac{\ln(r^{\frac{pq}{2p+q}} + r^{-\frac{pq}{2p+q}})}{2 \ln 2}. \quad (3.22)$$

The surface magnetization exponent depends on the amplitude of the coupling ratio r through λ_c as expected for a marginal sequence, but also on the layer widths. The variation of $\beta_s^{(m)}$ for several values of the parameters is shown in Fig. 2.

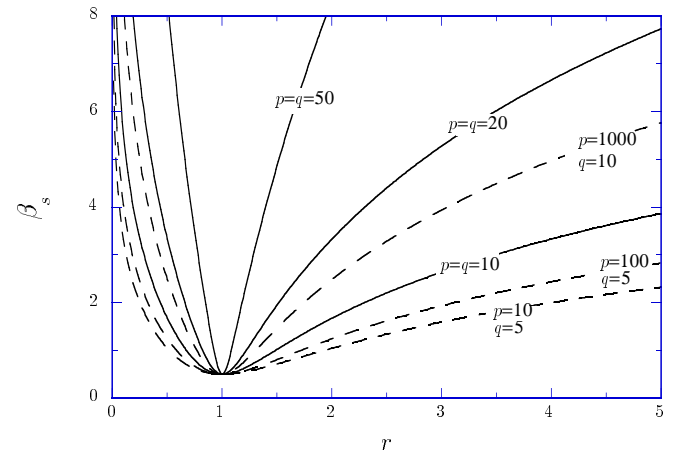


FIG. 2. Marginal variation of the surface magnetization exponent $\beta_s^{(m)}$ with the coupling ratio r for the period-doubling multilayer. The singularity is always weaker than in the homogeneous system and the surface transition is of second order for any value of r, p, q .

The analysis of the series (3.16) can be completed by a usual finite-size-scaling argument,³⁷ which implies that the following critical point behavior also holds: $\tilde{\Sigma}_L(0, \lambda_c) \sim L^{2x_{m_s}}$. The anomalous scaling dimension of the surface magnetization $x_{m_s} = \beta_s/\nu$ then takes the same value than β_s , and this requirement imposes that the correlation length exponent in the perturbed system keeps its unperturbed value $\nu = 1$. This property holds for any marginal sequence and can be understood within Luck's criterion, which has to remain valid in the perturbed system: the wandering exponent being constant, $\phi = 0$ indeed implies the constancy of ν .

In the case of the paper-folding sequence with $\rho_\infty = 1/2$, the critical point is determined by

$$\lambda_c = r^{-\frac{p}{p+q}}. \quad (3.23)$$

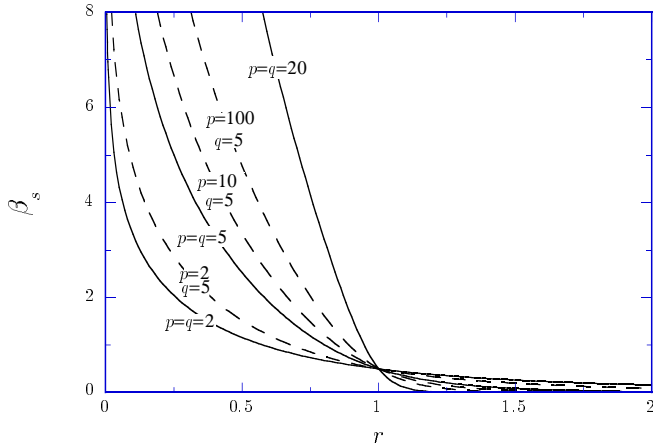


FIG. 3. Marginal variation of the surface magnetization exponent $\beta_s^{(m)}$ with the coupling ratio r for the paper-folding multilayer. The singularity is weakened by the perturbation when $r < 1$.

The same scaling analysis has been done in the case of the paper-folding sequence for the layered problem.²³ Translated to the multilayered problem, it leads to

$$\tilde{\Sigma}_{L=2^l}(0, \lambda_c) = (1 + \lambda_c^{2q})^l \sim (2^l)^{2\beta_s} \quad (3.24)$$

and to the surface exponent:

$$\beta_s(\lambda_c) = \frac{\ln(1 + \lambda_c^{2q})}{2 \ln 2} = \frac{\ln\left(1 + r^{-\frac{2pq}{p+q}}\right)}{2 \ln 2}, \quad (3.25)$$

whose variations are shown in Fig. 3. While period-doubling is a symmetric sequence where the relation $\beta_s^{(m)}(r, p, q) = \beta_s^{(m)}(r^{-1}, p, q)$ holds, it is not the case of the paper-folding perturbation for which the surface magnetic exponent has a monotonous variation. The singularity is thus weakened for $r < 1$ only. This result can be understood if one looks to the density of perturbed layers (of type p). Their density close to the surface is indeed larger than the asymptotic density ρ_∞ , leading to a weaker average coupling in the vicinity of the surface than in the bulk when $r < 1$. In the other regime $r > 1$, the average coupling close to the surface is enhanced and a stronger singularity follows.

IV. CROSSOVER IN MULTILAYERED ISING MODELS

The study of aperiodic multilayers does not present more difficulties than the usual layered systems, but it

can produce an interesting crossover in the critical behavior. While the perpendicular correlation length ξ_\perp is of the order of the size of the chain in the close neighborhood of the critical point, in which case the critical properties are governed by the aperiodic fixed point, this is no longer true when the system is moved far away from λ_c . In this latter situation, the correlation length decreases as λ increases and, at some point, becomes of the order of the first layer width p . The aperiodic structure of the system then becomes irrelevant and the behavior is controlled by the semi-infinite homogeneous fixed point, the unperturbed exponent $\beta_s = 1/2$ of the ordinary surface transition being recovered.³⁹

The evidence of this phenomenon appears immediately on a log-log plot as shown in Fig. 4 in the case of period-doubling sequence. The values of r and $p = q$ have been chosen for clearness in order to keep a constant value $\beta_s^{(m)} = 2$.

The surface magnetization can thus be written as follows:

$$m_s(t, p) = t^{1/2} f(p/\xi_\perp) \quad (4.1)$$

where $f(x)$ is a scaling function involving the relevant length scales which describe the surface behavior. It is shown on a log-log scale in Fig. 5 where $m_s t^{-1/2}$ is plotted against pt and $\xi_\perp \sim t^{-1}$.

For a fixed value of $\beta_s^{(m)}$, one obtains two different universal curves, one for $r > 1$ and the other for $r < 1$. This is due to the properties of the period-doubling sequence which allows to reach the same $\beta_s^{(m)} > 1/2$ with two different values of the coupling ratios r at fixed p and q values. The paper-folding sequence exhibits a rather different behavior shown in Fig. 6.

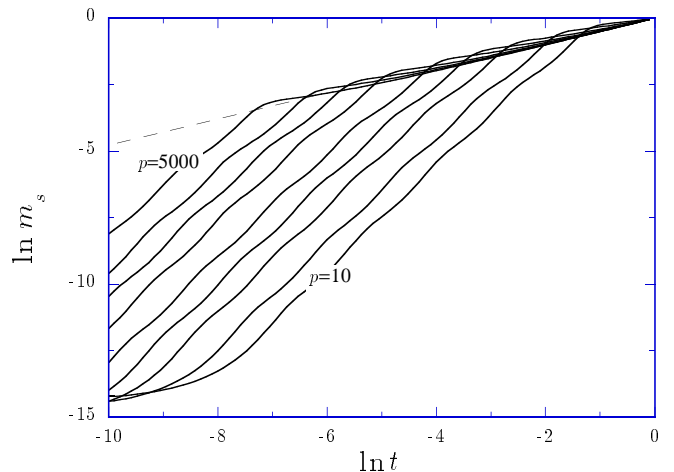


FIG. 4. Crossover between homogeneous fixed point ($\beta_s = 1/2$) towards aperiodic fixed point (here $\beta_s^{(m)} = 2$) when the critical point is approached (period-doubling sequence). The layer sizes are $p = q = 10$ ($r = 2.295$), $p = 20$ ($r = 1.515$), $p = 50$ ($r = 1.181$), $p = 100$ ($r = 1.087$), $p = 200$ ($r = 1.042$), $p = 500$ ($r = 1.017$), $p = 1000$ ($r = 1.008$), $p = 2000$ ($r = 1.004$) and $p = 5000$ ($r = 1.002$).

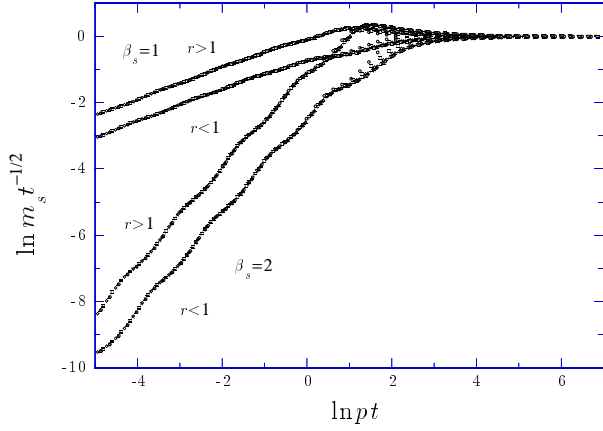


FIG. 5. Universal curves for the surface magnetization in the period-doubling sequence with $\beta_s^{(m)} = 2$ and 1 and $p = q = 10, 20, 50, 100, 200, 500, 1000, 2000, 5000$.

The scaling function of Eq. (4.1) has to satisfy appropriate asymptotic behaviors in order to provide a correct description of the two limiting power-law behaviors of m_s . Far away from $t = 0$ it has to keep a constant value (the usual surface magnetization amplitude of the homogeneous system) to agree with $m_s \sim t^{1/2}$. This requirement is satisfied in Fig. 5 and 6 and is responsible for the vanishing slopes for large values of pt . On the other hand, in order to recover the right varying exponent $\beta_s^{(m)}$ close to $t = 0$, the following power-law is expected in the vicinity of the critical point

$$f(x) \sim x^\theta, \quad x \rightarrow 0, \quad \theta = \frac{\beta_s^{(m)} - 1/2}{\nu}. \quad (4.2)$$

The average slopes calculated numerically in this second regime are in agreement with the expression of θ given above.

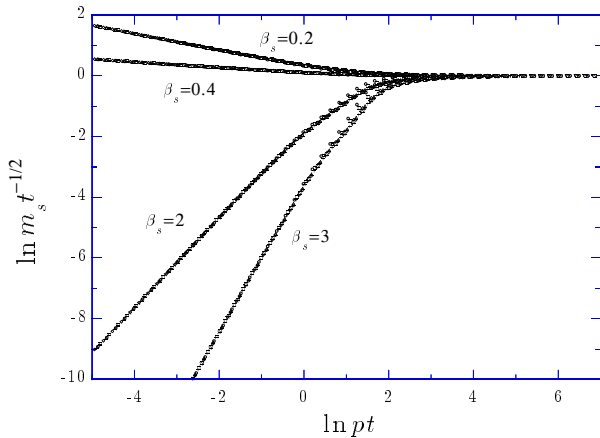


FIG. 6. Universal curves for the surface magnetization in the paper-folding sequence with $\beta_s^{(m)} = 3, 2, 0.4, 0.2$ and $p = q = 10, 20, 50, 100, 200, 500, 1000, 2000, 5000$.

The scaling functions shown in Figs. 5 and 6 exhibit a quite good agreement with the required asymptotic behaviors. In the homogeneous surface regime (far away from $t = 0$), this fact should be surprising since t is the deviation from the *aperiodic critical point*, given in Eq. (3.13). Introducing the homogeneous critical coupling $\lambda_{c,0} = r^{-1}$ of the first (perturbed) layer, and the corresponding deviation $t_0 = 1 - (\lambda r)^{-2}$, one has $t \simeq t_0(1 + \delta/t_0)$, where $\delta = 1 - r^2\lambda_c^2$ is a measure of the difference between the two critical point locations. Since δ is a small quantity in our calculations (for example $\delta \simeq 0.005$ in the case $p = q = 1000$, $r = 1.008$ in Fig. 5), we can expand Eq. (4.1) up to linear order in δ :

$$m_s(t, p) \sim t_0^{1/2} \left(1 + \frac{\delta}{2t_0} \right) f\left(\frac{p}{\xi_\perp}\right), \quad (4.3)$$

and there appears simply a correction to scaling term which is proportional to the difference between the two critical couplings. With the range of values used here, this correction to scaling term is negligible.

We can also point out log-periodic oscillations exhibited by the scaling function in the “aperiodic” regime.³⁸ This behavior is related to the discrete scale invariance of aperiodic sequences. The oscillating amplitude, A , is usually a periodic function of $\ln \xi_\perp / \ln m$ where m is the discrete scale factor (4 for period-doubling and 2 for paper-folding). In this multilayered system, the correlation length is naturally measured in units of p such that the scaling function in the neighborhood of the critical point can be rewritten

$$f(x) \sim A(\ln x / \ln m) x^\theta, \quad (4.4)$$

leading to

$$\ln f(x) \sim \ln[A(\ln x / \ln m)] + \theta \ln x. \quad (4.5)$$

in agreement with the oscillations around an average slope θ .

V. CORRELATION LENGTH AND MARGINAL ANISOTROPY

In Ref. 23, the low-energy excitation behavior has been studied for the layered problem, leading to a finite-size power law at the critical point involving an anisotropy exponent z . The conjecture

$$z = x_{m_s} + \bar{x}_{m_s}, \quad (5.1)$$

was proposed,⁴⁰ and it has then been proved for specific sequences, using renormalization group calculations.⁴¹ and has furthermore been supported for an arbitrary marginal perturbation by an approximate calculation of $\varepsilon_1(L)$,⁴² leading to $\varepsilon_1(L) \sim m_s(L) \bar{m}_s(L) \prod_{i=1}^{L-1} \lambda_i^{-1}$ from which Eq. (5.1) follows. Moreover, the constancy of the

correlation exponent in the perturbed systems has been obtained exactly in Ref. 41,42

Assuming the same finite-size behavior for the first component of the eigenvectors corresponding to the two lowest excitations, $\Phi_1(1) \sim \Phi_2(1) \sim L^{-x_{ms}}$, the surface energy density exponent also follows

$$x_{e_s} = z + 2x_{m_s}. \quad (5.2)$$

The correspondence between the classical two-dimensional system and the quantum chain shows that the correlation length in the Euclidean time direction (along the layers) is given by the inverse of the smallest non-vanishing gap in the Hamiltonian spectrum, *i.e.* $\xi_{\parallel} = 1/\varepsilon_1$ at λ_c . In the low-temperature phase $\lambda > \lambda_c$, the lowest excitation ε_1 vanishes exponentially due to the asymptotic degeneracy of the ferromagnetic ground state in the thermodynamic limit, and the parallel correlation length is thus given by the next fermion excitation:

$$\xi_{\parallel} = \frac{1}{\varepsilon_2}. \quad (5.3)$$

In the previous sections, we found the marginal behavior of the surface magnetization at the aperiodic critical point, and its crossover towards the usual ordinary surface transition fixed point in the ordered phase. We can expect here, as in the usual layered problem, a strong anisotropic scaling behaviour responsible for a special behavior of ξ_{\parallel} at the aperiodic fixed point. It can be studied through the temperature dependence when $\lambda > \lambda_c$ (*via* ε_2) or by finite-size scaling at the critical point $\lambda = \lambda_c$ (*via* ε_1).

With free boundary conditions, the system (2.3) can be rewritten in a matrix form $(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B})\Phi_{\alpha} = \varepsilon_{\alpha}^2 \Phi_{\alpha}$. Here, the standard notation has been used.³⁰ Due to the tridiagonal structure of the “excitation matrix” $(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B})$, the recursion relations for the components of Φ_{α} take the form:⁴³

$$\begin{aligned} \begin{pmatrix} \Phi_{\alpha}(l) \\ \Phi_{\alpha}(l+1) \end{pmatrix} &= \mathbf{T}_l \begin{pmatrix} \Phi_{\alpha}(l-1) \\ \Phi_{\alpha}(l) \end{pmatrix}, \\ &= \begin{pmatrix} 0 & 1 \\ s_l & t_l(\varepsilon_{\alpha}) \end{pmatrix} \begin{pmatrix} \Phi_{\alpha}(l-1) \\ \Phi_{\alpha}(l) \end{pmatrix} \end{aligned} \quad (5.4)$$

with

$$s_l = -\frac{\lambda_{l-1}}{\lambda_l}, \quad t_l(\varepsilon_{\alpha}) = \frac{\varepsilon_{\alpha}^2 - 1 - \lambda_{l-1}^2}{\lambda_l}, \quad 2 \leq l \leq L-1 \quad (5.5)$$

and boundary terms

$$\begin{aligned} \begin{pmatrix} \Phi_{\alpha}(1) \\ \Phi_{\alpha}(2) \end{pmatrix} &= \mathbf{T}_1 \begin{pmatrix} \Phi_{\alpha}(0) \\ \Phi_{\alpha}(1) \end{pmatrix}, \\ \begin{pmatrix} \Phi_{\alpha}(L) \\ \lambda_L \Phi_{\alpha}(L+1) \end{pmatrix} &= \mathbf{T}_L \begin{pmatrix} \Phi_{\alpha}(L-1) \\ \Phi_{\alpha}(L) \end{pmatrix}, \end{aligned} \quad (5.6)$$

$$\begin{aligned} \Phi_{\alpha}(0) &= 0 \\ \lambda_L \Phi_{\alpha}(L+1) &= 0. \end{aligned} \quad (5.7)$$

Finally, one has

$$\begin{pmatrix} \Phi_{\alpha}(L) \\ f(\varepsilon) \end{pmatrix} = \mathbf{T}_L \dots \mathbf{T}_2 \mathbf{T}_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \mathbf{M}_L \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (5.8)$$

where the eigenvectors are not normalized at this step and the excitation energies are deduced from the positive zeroes of $f(\varepsilon)$. In a multilayered structure, within a given layer of size p , the same matrix appears $p-1$ times and in the case $p=q$, Eq. (5.8) becomes

$$\begin{aligned} \mathbf{M}_L &= \mathbf{T}_L (\mathbf{P}_{f_L})^{p-2} \mathbf{Q}_{f_L, f_{L-1}} (\mathbf{P}_{f_{L-1}})^{p-1} \dots \\ &\dots \mathbf{Q}_{f_3, f_2} (\mathbf{P}_{f_2})^{p-1} \mathbf{Q}_{f_2, f_1} (\mathbf{P}_{f_1})^{p-1} \mathbf{T}_1 \end{aligned} \quad (5.9)$$

where \mathbf{P}_{f_k} is a “propagation” matrix inside layer k and $\mathbf{Q}_{f_{k+1}, f_k}$ a “transfer matrix” from layer k to layer $k+1$. We can easily give a closed form for the propagation terms:

$$\mathbf{P}_{f_k} = \begin{pmatrix} 0 & 1 \\ -1 & t_k(\varepsilon) \end{pmatrix}, \quad (5.10)$$

after diagonalization, leads to

$$(\mathbf{P}_{f_k})^{p-1} = \mathbf{S}_{f_k} \begin{pmatrix} \alpha_+^{p-1} & 0 \\ 0 & \alpha_-^{p-1} \end{pmatrix} \mathbf{S}_{f_k}^{-1} \quad (5.11)$$

where α_{\pm} are the eigenvalues of \mathbf{P}_{f_k} and \mathbf{S}_{f_k} the changing of basis matrix.

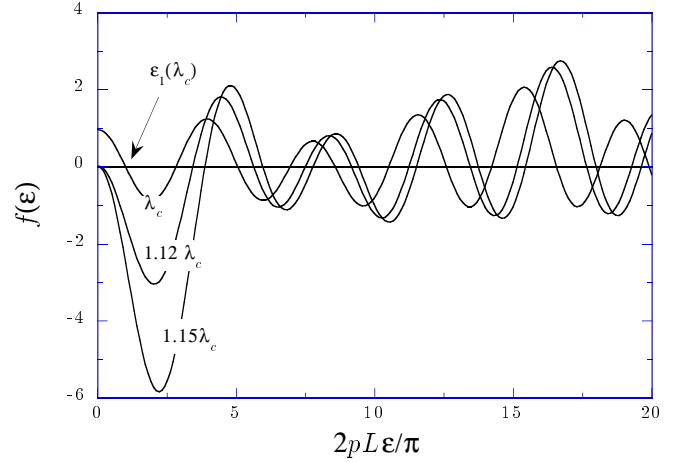


FIG. 7. Typical shape of the function $f(\varepsilon)$ for period-doubling sequence, with $L = 2^4$, $p = q = 2$, $r = 1.1$, and several values of λ in the ordered phase.

It is now possible to get \mathbf{M}_L for any value of the layer sizes p , and, in the case of large values of p , this technique is quite efficient compared to a direct diagonalization of the excitation matrix. Some numerical troubles can nevertheless occur, since the function $f(\varepsilon)$ exhibits oscillations whose amplitude increases sharply with the sizes L

and p while the period decreases rapidly. An example is shown in Fig. 7 for a small size. It is clear from Fig. 7 that, as λ increases from its critical value, the lowest excitation ε_1 decreases while the next one, ε_2 , increases. The temperature behaviour of ξ_{\parallel} is in agreement with a modified power-law $\xi_{\parallel} \sim t^{-z}$, where the anisotropy exponent z is assumed to be the sum

$$z(r, p, q) = \beta_s^{(m)}(r, p, q) + \beta_s^{(m)}(r^{-1}, p, q) \quad (5.12)$$

as in the layered system. The temperature dependence of ε_2^{-1} is shown on a log-log scale in Fig. 8 in the ordered phase $\lambda > \lambda_c$. From the linear behavior, we can obtain the anisotropy exponent z . The numerical results deduced from the slopes of the asymptotic linear behavior are given in Tab. I. The numerical data are in agreement with Eq. (5.12).

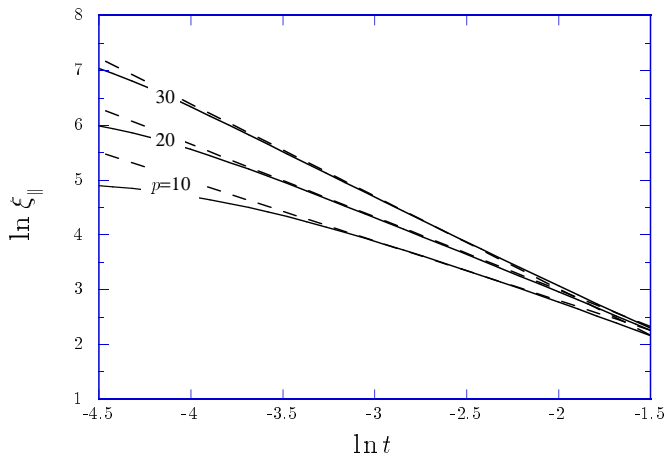


FIG. 8. Temperature dependence of the parallel correlation length on a log-log scale in the ordered phase $\lambda > \lambda_c$. The deviation from the asymptotic linear behavior (dashed lines) when $t \rightarrow 0$ is a finite size effect.

TABLE I. Parallel correlation length exponent ν_{\parallel} , deduced from the slopes of log-log plots of ξ_{\parallel} v.s. t , compared to the anisotropy exponent z for the period-doubling sequence.

r	$p = q$	ν_{\parallel}	z
1.1	10	1.102	1.072
1.1	20	1.286	1.273
1.1	30	1.493	1.575
0.9	10	1.099	1.087
0.9	20	1.334	1.330
0.9	30	1.626	1.686

A finite-size-scaling study provides an alternate numerical calculation of these exponents.

It has been done in Tab. II for the anisotropy exponent, but also for the surface magnetization and energy density exponents, in order to check the conjecture (5.2) for the multilayered system. The layer widths have been limited to small values in order to reach large enough

values of L (2^{10} for the period doubling sequence for example) and extrapolation to infinite size has been performed, using the BST algorithm, which is efficient for finite-size-scaling analyses.⁴⁴

TABLE II. Anisotropy, surface magnetization and surface energy density exponents deduced from a finite-size-scaling study for the period-doubling sequence.

r	$p = q$	z		$x_{m_s}^{(m)}$		$x_{e_s}^{(m)}$	
		num.	theor.	num.	theor.	num.	theor.
2	2	1.15(2)	1.149	.58(3)	.574	2.29(1)	2.298
2	3	1.33(2)	1.322	.69(5)	.661	2.62(3)	2.644
3	2	1.36(2)	1.357	.70(4)	.678	2.70(2)	2.713
3	3	1.75(2)	1.737	.90(4)	.869	3.45(2)	3.474

VI. CONCLUSION

We have presented the study of the influence of layer widths p and q in aperiodic multilayered Ising models. The perturbations under consideration correspond to vanishing wandering exponents, and thus lead to marginal critical behaviors in the two-dimensional Ising model. From a finite-size scaling analysis of the aperiodic series which defines the surface magnetization, we obtained the corresponding critical exponents which continuously vary with the modulation ratio. This defines the *aperiodic fixed point behavior* characterized by an anisotropic scaling which has been studied numerically.

When the system, in the ordered phase, is moved away from this critical point, the surface magnetization exhibits a crossover towards another regime, governed by the ordinary surface transition fixed point. We have shown that the crossover is well described by scaling functions of a single scaled variable which obey well-defined asymptotic behaviors.

Aperiodic multilayers are now feasible by molecular beam epitaxy,⁴⁵ and although nothing experimental has been done up to now to study the critical behavior of such systems, crossover effects between the two regimes should be experimentally observable.

One should finally mention that the same type of study for relevant aperiodic modulations would be interesting especially when an enhancement of the modified couplings close to the surface leads to first order surface transitions in a two-dimensional system. This will be the subject of a further investigation.

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- ‡ The Laboratoire de Physique des Matériaux is Unité de Recherche Associée au C.N.R.S. No 155.
- ¹ D. Schechtman, I. Blech, D. Gratias, and J.W. Cahn, Phys. Rev. Lett. **53**, 1951 (1984)
 - ² U. Grimm and M. Baake, cond-mat/9604116 (1996)
 - ³ B.M. McCoy and T.T. Wu Phys. Rev. Lett. **21**, 549 (1968)
 - ⁴ B.M. McCoy and T.T. Wu Phys. Rev. **176**, 631 (1968)
 - ⁵ B.M. McCoy Phys. Rev. B **2**, 2795 (1970)
 - ⁶ H. Au-Yang and B.M. McCoy Phys. Rev. B **10**, 886 (1974)
 - ⁷ F. Iglói, J. Phys. A **21**, L911 (1988)
 - ⁸ M.M. Doria and I.I. Satija, Phys. Rev. Lett. **60**, 444 (1988)
 - ⁹ V.G. Benza, Europhys. Lett. **8**, 321 (1989)
 - ¹⁰ M. Henkel and A. Patkós, J. Phys. A **25**, 5223 (1992)
 - ¹¹ Z. Lin and R. Tao, J. Phys. A **25**, 2483 (1992)
 - ¹² L. Turban and B. Berche, Z. Phys. B **92**, 307 (1993)
 - ¹³ C.A. Tracy, J. Phys. A **21**, L603 (1988)
 - ¹⁴ J. M. Luck, J. Stat. Phys. **72**, 417 (1993).
 - ¹⁵ A.B. Harris, J. Phys. C **7**, 1671 (1974)
 - ¹⁶ M. Queffélec, “Substitution Dynamical Systems”, Lecture Notes in Mathematics Vol. **1294**, A. Dold and B. Eckmann eds. (Springer, Berlin, 1987) p. 97.
 - ¹⁷ J. M. Dumont, in *Number Theory and Physics*, Springer Proceedings in Physics, Vol. 47, edited by J. M. Luck, P. Moussa, and M. Waldschmidt (Springer, Berlin, 1990), p. 185.
 - ¹⁸ L. Turban, F. Iglói, and B. Berche, Phys. Rev. B **49**, 12695 (1994).
 - ¹⁹ F. Iglói and L. Turban, Europhys. Lett. **27**, 91 (1994)
 - ²⁰ L. Turban, P. E. Berche, and B. Berche, J. Phys. A **27**, 6349 (1994).
 - ²¹ D. Karevski, G. Palàgyi, and L. Turban, J. Phys. A **28**, 45 (1995)
 - ²² B. Berche *et al.*, J. Phys. A **28**, L165 (1995)
 - ²³ P. E. Berche, B. Berche, and L. Turban, J. Phys. I (France) **6**, 621 (1996).
 - ²⁴ F. Iglói and P. Lajkó, J. Phys. A **29**, 4803 (1996)
 - ²⁵ F. Iglói, P. Lajkó, and F. Szalma, Phys. Rev. B **52**, 7159 (1995)
 - ²⁶ D. B. Abraham, Stud. appl. Math. **50**, 71
 - ²⁷ J. Kogut, Rev. Mod. Phys. **51**, 659 (1979).
 - ²⁸ P. Pfeuty, Ann. Phys. **57**, 79 (1970).
 - ²⁹ P. Jordan and E. Wigner, Z. Phys. **47**, 631 (1928).
 - ³⁰ E. H. Lieb, T.D. Schultz, and D. C. Mattis, Ann. Phys. NY, **16**, 406 (1961).
 - ³¹ P. Pfeuty, Phys. Lett. **72A**, 245 (1979).
 - ³² P. Collet and J. P. Eckmann, “Iterated Maps on the Interval as Dynamical Systems” (Birkhäuser, Boston, 1980).
 - ³³ M. Dekking, M. Mendès-France, and A. van der Poorten, Math. Intelligencer **4**, 130 (1983).
 - ³⁴ I. Peschel, Phys. Rev. B **30**, 6783 (1984).
 - ³⁵ The deviation t from the critical point is defined as a positive quantity in the ordered phase.
 - ³⁶ F. Iglói, J. Phys. A **19**, 3077 (1986).
 - ³⁷ M. N. Barber, “Phase Transitions and Critical Phenomena”, Vol. **8**, C. Domb and J.L. Lebowitz eds (Academic Press, London, 1983) p. 145.
 - ³⁸ D. Karevski and L. Turban, J. Phys. A **29**, 3461 (1996).
 - ³⁹ K. Binder, “Phase Transitions and Critical Phenomena”, Vol. **8**, C. Domb and J.L. Lebowitz eds (Academic Press, London, 1983) p. 1.
 - ⁴⁰ This relation states that z is given by the sum of the scaling dimensions associated to the left ($x_{m_s}(\lambda_c)$) and the right surfaces ($\bar{x}_{m_s}(\lambda_c) = x_{m_s}(\lambda_c^{-1})$), the latter one being deduced from the former by the transformation $r \rightarrow r^{-1}$, which is equivalent to $\lambda_c \rightarrow \lambda_c^{-1}$.
 - ⁴¹ F. Iglói and L. Turban, Phys. Rev. Lett. **77**, 1206 (1996).
 - ⁴² F. Iglói, L. Turban, D. Karevski, and F. Szalma, to be published
 - ⁴³ H. Schmidt, Phys. Rev. **105**, 425 (1957).
 - ⁴⁴ M. Henkel and G. Schütz, J. Phys. A **21**, 2617 (1988).
 - ⁴⁵ C.F. Majkrzak *et al.*, Adv. Phys. **40**, 99 (1991)